APPROACH TO MODEL BASED REACTOR OPTIMIZATION WITH PACKED POCS FOR A HETEROGENEOUSLY CATALYZED EXTREMELY FAST HIGHLY ENDOTHERMAL REACTION

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Abstract

This contribution investigates the process intensification of an extremely fast highly endothermal reaction in a tubular reactor. For this purpose, the multi-level reactor design (MLRD) methodology (Freund et al., 2019, Peschel et al., 2010) was applied to an exemplary reaction system. To determine the optimal reaction conditions leading to an increased productivity, the optimization must include the intrinsic reaction kinetics. Therefore, a dedicated laboratory reactor setup was developed to ensure measurements in the kinetic regime, unbiased from external mass or heat transfer limitations. The latter has proven to be the limiting factor in the industrial process. To address the heat transfer challenge, packed POCS are investigated in this study as a means of increasing the heat transport into the catalyst bed (Ambrosetti et al., 2020). The following model based reactor optimization is based on a reactor model of packed POCS in a tubular reactor including the intrinsic reaction kinetics.

Keywords

Endothermal Reaction, Multi-Level Reactor Design, Packed POCS

Introduction

Process intensification and optimization of industrial plants in the chemical process industries is key for the implementation of more energy efficient processes with reduced carbon dioxide emissions at increased productivity. For this purpose, the design and optimization of the reactor as central process unit must aim at achieving optimal reaction conditions along the reaction route. In this regard, the multi-level reactor design (MLRD) methodology (Freund et al., 2019, Peschel et al., 2010) has proven to be a suitable approach and therefore was applied in this study on the example of an extremely fast highly endothermal reaction. The aim was to optimize the existing industrial process to achieve a higher space-time-yield with a more energy efficient reactor concept, thereby also reducing the carbon dioxide footprint.

In catalytic tubular reactors, suitable reaction conditions along the reactor axis can be realized by different options. One promising approach is the use of novel catalyst supports, and particularly of so called Periodic Open Cellular Structures (POCS) as introduced by Freund and Schwieger (Inayat et al., 2011). To maximize catalyst inventory in the reactor, a combination of POCS with high void fraction with catalyst pellets in the

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void space, known as packed POCS (Ambrosetti et al., 2020), is investigated in this study.

The bottleneck of this extremely fast highly endothermal reaction is the heat transfer into the catalyst bed. The high endothermicity of the reaction can result in cold spots in the catalyst bed leading to a decrease in reaction rate and thereby to a lower productivity. Therefore, the goal of process intensification is to determine a method to increase the heat transport into the catalyst bed and to define optimal reaction conditions to achieve a high space-time-yield. For this purpose, in the present study a reaction kinetic model is established based on data from extensive measurements and implemented in the multi-level reactor design approach.

Multi-Level Reactor Design: Intrinsic Reaction Kinetics Measurements

In the first step of the MLRD methodology, the optimal reaction conditions for exemplary reaction are determined using the intrinsic reaction kinetics in the optimization. To handle the challenges in kinetic measurements for extremely fast highly endothermal reactions, high weight hourly space velocities (WHSV) are necessary to ensure measurements in the kinetic regime, unbiased from external mass or heat transfer limitations. For this purpose, a dedicated lab plant setup with a Berty-type reactor, which exhibits approximately ideal behavior at high volume flows inside the reactor, was designed and built. The composition of the product stream was analyzed with a micro gas chromatograph, allowing for a high precision analysis at relativley high temporal resolution. With this dedicated experimental setup, extensive kinetic measurements over a wide range of reaction conditions were performed. Afterwards, parameter estimation for the reaction kinetic model was carried out, resulting in an intrinsic reaction kinetics model enabling the determination of optimal reaction conditions using MLRD.

Optimization with Packed POCS

The high thermal conductivity of the continuous structure of POCS improves the heat transport compared to conventional randomly packed beds and results in a more homogeneous temperature distribution along the reactor axis (Ambrosetti et al., 2020). Therefore, a reactor model containing correlations describing the heat transport within the packed POCS as well as the pressure drop along the reactor were implemented. The simulated concentration and temperature profiles along the reactor were compared to the results of the reactor model of the industrial reactor, which serves as a reference case. A following optimization study was performed using the reactor model of the tubulur reactor with packed POCS. The objective of the optimization was to achieve an approximately isothermal temperature profile along the reactor and thereby ensuring a higher space-time-yield than in the industrial process.

Conclusions

The MLRD approach resulted in a reactor design for approaching the optimal reaction conditions. Inserting packed POCS into the tubular reactor leads to a significantly enhanced heat transfer compared to a conventional randomly packed bed. This results in a decrease of the temperature drop at the cold spot (see Figure 1) and to a higher temperature level at the reactor outlet. Consequently, a higher overall conversion is reached, thereby significantly increasing the productivity and the energy efficiency of the process.

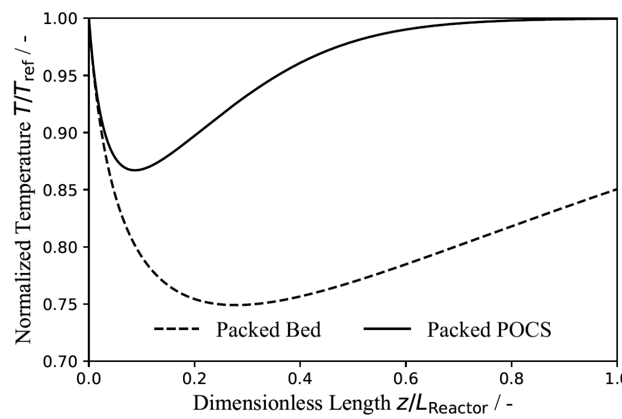

Figure 1. Comparison of the axial temperature profile in the packed bed (dotted line) and the packed POCS (solid line)

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